

PTO/SB/08a (09-08)

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| Substitute for form 1449/PTO <h2 style="text-align: center;">INFORMATION DISCLOSURE STATEMENT BY APPLICANT</h2> <p style="text-align: center;">(Use as many sheets as necessary)</p> | | Complete if Known Application Number: 09/502,133-Conf. #4787 Filing Date: February 11, 2000 First Named Inventor: Harold E. HELSON Art Unit: 2128 Examiner Name: H. M. Jones Attorney Docket Number: 0103544.00131US2 | |
| Sheet | 2 | of | 5 |

| NON PATENT LITERATURE DOCUMENTS | | | |
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| | CA | BALASUBRAMANIAN, K. J., "Computer Perception of Molecular Symmetry", <i>J. Chem. Inf. Comput. Sci.</i> , Vol. 35, pp. 761-770, 1995 | |
| | CB | BALDUCCI, R. et al., "Efficient Exact Solution of the Ring Perception Problem", <i>J. Chem. Inf. Comput. Sci.</i> , Vol. 34, pp. 822-831, 1994 | |
| | CC | BAUER, J. et al., "IGOR and RAIN - The First Mathematically Based Multi-Purpose Problem-Solving Computer Programs for Chemistry and Their Use as Generators of Constitutional Formulas", <i>Informal Commun. Math. Chem. (MATCH)</i> , No. 27, pp. 31-47, 1992 | |
| | CD | BAYADA, D. M. et al., "An Algorithm for the Multiple Common Subgraph Problem", <i>J. Chem. Inf. Comput. Sci.</i> , Vol. 32, pp. 680-685, 1992 | |
| | CE | BENECKE, C. et al., "MOLGEN, a generator of connectivity isomers and stereoisomers for molecular structure elucidation", <i>Anal. Chim. Acta</i> , Vol. 314, pp. 141-147, 1995 | |
| | CF | BERTRAND, A. et al., "DESMOL: a Subroutine for the Generation of Molecular Structures with Stereochemical Information from Connectivity Data", <i>J. Chem. Res. (S)</i> , p. 158, 1994 | |
| | CG | BLEY, K. et al., "Constitutional Formulae generated from Connectivity Information: the Program MDRAW", <i>J. Chem. Res. (S)</i> , p. 261, 1991 | |
| | CH | CARHART, R. E., "A Model-Based Approach to the Teletype Printing of Chemical Structures", <i>J. Chem. Inf. Comput. Sci.</i> , Vol. 16, No. 2, pp. 82-88, 1976 | |
| | CI | ChemDraw Chemical Structure Drawing Standard, <i>User's Guide</i> , CS Chem3D 4.0 for Windows and Macintosh, CambridgeSoft Corporation, 1986-1997 | |
| | CJ | DALBY, J. et al., "Description of Several Chemical Structure File Formats Used by Computer Programs Developed at Molecular Design Limited", <i>J. Chem. Inf. Comput. Sci.</i> , Vol. 32, pp. 244-255, 1992 | |

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| | | Filing Date | February 11, 2000 | | |
| | | First Named Inventor | Harold E. HELSON | | |
| | | Art Unit | 2128 | | |
| | | Examiner Name | H. M. Jones | | |
| | | Attorney Docket Number | 0103544.00131US2 | | |

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| | CK | DITTMAR, P.G. et al., "An Algorithmic Computer Graphics Program for Generating Chemical Structure Diagrams", <i>J. Chem. Inf. Comput. Sci.</i> , Vol. 17, No. 3, pp. 186-192, 1977 | | |
| | CL | DOWNS, G.M. et al., "Review of Ring Perception Algorithms for Chemical Graphs", <i>J. Chem. Inf. Comput. Sci.</i> , Vol. 29, pp. 172-187, 1989 | | |
| | CM | FIGUERAS, J. et al., "Automorphism and Equivalence Classes", <i>J. Chem. Inf. Comput. Sci.</i> , Vol. 32, pp. 153-157, 1992 | | |
| | CN | FIGUERAS, J., "Ring Perception Using Breadth-First Search", <i>J. Chem. Inf. Comput. Sci.</i> , Vol. 36, p. 986-991, 1996 | | |
| | CO | FREREJACQUE, M., "No. 108 - Condensation d'une molecule organique", <i>Bull. Soc. Chim. Fr., (Memoires)</i> , Vol. 5, pp. 1008-1011, 1939 | | |
| | CP | GOTHE, S.A. et al., "Computer-Assisted Mechanistic Evaluation of Organic Reactions. 22. The Generation and Use of Three-Dimensional Structures", <i>J. Org. Chem.</i> , Vol. 58, pp. 5081-5094, 1993 | | |
| | CQ | HELSON, "Structure Diagram Generation", <i>Reviews in Computational Chemistry</i> , Vol. 13, Ch. 6, pp. 313-398, 1999 | | |
| | CR | JUDSON, R., "Genetic Algorithms and Their Use in Chemistry", <i>Reviews of Computational Chemistry</i> , Ch. 1, Vol. 10, pp. 1-73, 1997 | | |
| | CS | LIETH, C.v.d. et al., "RINGS - a general program to build ring systems", <i>J. Mol. Graphics</i> , Vol. 2, pp. 117-123, 1984 | | |
| | CT | MOLCHANOVA, M.S. et al., "Computer Generation of Molecular Structures by the SMOG Program", <i>J. Chem. Inf. Comput. Sci.</i> , Vol. 36, pp. 888-899, 1996 | | |

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| | CU | RAYNER, J.D. et al., "A Concise Connection Table Based on Systematic Nomenclatural Terms", <i>J. Mol. Graphics</i> , Vol. 1, pp. 108-111, 1983 | |
| | CV | RUSINKO, A. et al., "Using CONCORD to Construct a Large Database of Three-Dimensional Coordinates from Connection Tables", <i>J. Chem. Inf. Comput. Sci.</i> , Vol. 29, p. 251-255, 1989 | |
| | CW | SADOWSKI, J. et al., "Comparison of Automatic Three-Dimensional Model Builders Using 639 X-ray Structures", <i>J. Chem. Inf. Comput. Sci.</i> , Vol. 34, p. 1000-1008, 1995 | |
| | CX | SHELLEY, C.A., "Heuristic Approach for Displaying Chemical Structures", <i>J. Chem. Inf. Comput. Sci.</i> , Vol. 23, pp. 61-65, 1983 | |
| | CY | SHMUELI, U., "Simple and efficient approach to preparation of molecular drawings", <i>J. Mol. Graphics</i> , Vol. 2, pp. 111-112, 1984 | |
| | CZ | THOMSON, L.G. et al., "Organic Search and Display Using a Connectivity Matrix Derived from Wiswesser Notation", <i>J. Chem. Doc.</i> , Vol. 7, pp. 204-209, November 1967 | |
| | CA1 | WEININGER, D., "SMILES, a Chemical Language and Information System. 1. Introduction to Methodology and Encoding Rules", <i>J. Chem. Inf. Comput. Sci.</i> , Vol. 28, pp. 31-36, 1988 | |
| | CB1 | WEININGER, D., "Smiles. 3. Depict. Graphical Depiction of Chemical Structures", <i>J. Chem. Inf. Comput. Sci.</i> , Vol. 30, pp. 237-243, 1990 | |
| | CC1 | WIPKE, T., "AIMB: Analogy and Intelligence in Model Building. System Description and Performance Characteristics", <i>Computer Representation and Manipulation of Chemical Information</i> , pp. 147-174, Wipke et al. editors, Krieger, NY, 1981 | |
| | CD1 | WIPKE, W. T. et al., "Computer-Assisted Three-Dimensional Synthetic Analysis", <i>Tet. Comput. Method.</i> , Vol. 1, pp. 147-174, 1988 | |

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